

## Author index to volume 218

- Alikhani, M.E., see Tremblay, B. 218 (1997) 37
- Alonso, J.L., F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler, Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex 218 (1997) 267
- Antoine, R., see Dugourd, Ph. 218 (1997) 163
- Au, J.W. and C.E. Brion, Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide 218 (1997) 109
- Au, J.W. and C.E. Brion, Quantitative studies of the photoabsorption and photoionization of  $\text{PCl}_3$  in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions 218 (1997) 87
- Bagnich, S.A., The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses 218 (1997) 277
- Boilot, J.P., see Brunel, M. 218 (1997) 301
- Borsenberger, P.M., see Sinicropi, J.A. 218 (1997) 331
- Brion, C.E., see Au, J.W. 218 (1997) 109
- Brion, C.E., see Au, J.W. 218 (1997) 87
- Brion, C.E., see Olney, T.N. 218 (1997) 127
- Broyer, M., see Dugourd, Ph. 218 (1997) 163
- Brun, A., see Brunel, M. 218 (1997) 301
- Brunel, M., F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun, Reverse saturable absorption in palladium and zinc tetraphenyltetraabenzoporphyrin doped xerogels 218 (1997) 301
- Buijsse, B., see Wouters, E.R. 218 (1997) 309
- Buonomo, E., F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal, A full quantum study of the vibrational predissociation mechanisms in  $\text{Ar}_3^+$  cluster 218 (1997) 71
- Burton, G.R., see Olney, T.N. 218 (1997) 127
- Campagne, B., see Brunel, M. 218 (1997) 301
- Canva, M., see Brunel, M. 218 (1997) 301
- Chan, W.F., see Olney, T.N. 218 (1997) 127
- Chaput, F., see Brunel, M. 218 (1997) 301
- Chowdhury, P.K., see Schmid, R.P. 218 (1997) 291
- Christen, C., see Dietz, F. 218 (1997) 43
- Chua, M. and P.A. Tanner, Direct calculation of electronic Raman scattering intensity for  $\text{Ce}^{3+}$  in  $\text{Cs}_2\text{NaCeCl}_6$  218 (1997) 83
- Cooper, G., see Olney, T.N. 218 (1997) 127

- Cowdery-Corvan, J.R., see Sinicropi, J.A. 218 (1997) 331
- Cuadros, F., A. Mulero and W. Okrasinski, Thermodynamic shift from three- to two-dimensional systems 218 (1997) 235
- Delgado-Barrio, G., see Buonomo, E. 218 (1997) 71
- DeWitt, M.J., D.W. Peters and R.J. Levis, Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation 218 (1997) 211
- Dietz, F., N. Tyutyulkov, C. Christen and K. Lüders, Nature of the magnetic interaction of Wurster's radicals in the solid state 218 (1997) 43
- Ding, S., see Guan, D. 218 (1997) 1
- Dreizler, H., see Alonso, J.L. 218 (1997) 267
- Dugourd, Ph., D. Rayane, R. Antoine and M. Broyer, Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process 218 (1997) 163
- Dyke, J.M., see Mack, P. 218 (1997) 243
- Evangelisti, S., Carbon-oxygen clusters as hypothetical high energy-density materials 218 (1997) 21
- Fišer, J., see Vojtík, J. 218 (1997) 13
- Gianturco, F.A., see Buonomo, E. 218 (1997) 71
- Guan, D., X. Yi, S. Ding and B. Yang, Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface 218 (1997) 1
- Hawlicka, E. and D. Swiatla-Wojcik, Molecular dynamics simulation of NaCl solutions in methanol-water mixtures. Intramolecular vibrations of the solvent components 218 (1997) 49
- Hirao, K., see Tajima, N. 218 (1997) 257
- Hiraya, A., see Kanda, K. 218 (1997) 199
- Hu, Y., W. Lu and S. Yang, Intermolecular vibrations of the van der Waals complex  $p\text{-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$  218 (1997) 325
- Ito, F., see Schmid, R.P. 218 (1997) 291
- Jones, H., see Schmid, R.P. 218 (1997) 291
- Kanda, K., S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake, Photodissociation spectroscopy of ICN in the vacuum ultraviolet region 218 (1997) 199
- Katsumata, S., see Kanda, K. 218 (1997) 199
- Kondow, T., see Kanda, K. 218 (1997) 199
- Küster, J., see Schael, F. 218 (1997) 175
- Lesarri, A., see Alonso, J.L. 218 (1997) 267
- Levis, R.J., see DeWitt, M.J. 218 (1997) 211
- Löhmansröben, H.-G., see Schael, F. 218 (1997) 175
- López, J.C., see Alonso, J.L. 218 (1997) 267
- Lorenzo, F.J., see Alonso, J.L. 218 (1997) 267
- Lu, W., see Hu, Y. 218 (1997) 325
- Lüders, K., see Dietz, F. 218 (1997) 43

- Mack, P., J.M. Dyke and T.G. Wright, Calculated thermodynamics of reactions involving  $\text{NO}^+ \cdot \text{X}$  complexes (where  $\text{X} = \text{H}_2\text{O}$ ,  $\text{N}_2$  and  $\text{CO}_2$ ) 218 (1997) 243
- Magin, E.H., see Sinicropi, J.A. 218 (1997) 331
- Manceron, L., see Tremblay, B. 218 (1997) 37
- Mata, S., see Alonso, J.L. 218 (1997) 267
- Mataras, D., see Stamou, S. 218 (1997) 57
- Maus, M. and W. Rettig, The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds 218 (1997) 151
- Mets, Ü., J. Widengren and R. Rigler, Application of the antibunching in dye fluorescence: measuring the excitation rates in solution 218 (1997) 191
- Miret-Artés, S., see Buonomo, E. 218 (1997) 71
- Miyawaki, J., see Schmid, R.P. 218 (1997) 291
- Mulero, A., see Cuadros, F. 218 (1997) 235
- Nagata, T., see Kanda, K. 218 (1997) 199
- Nakanaga, T., see Schmid, R.P. 218 (1997) 291
- Okrasinski, W., see Cuadros, F. 218 (1997) 235
- Olney, T.N., G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan, Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique 218 (1997) 127
- Peters, D.W., see DeWitt, M.J. 218 (1997) 211
- Pilar de Lara, M., see Buonomo, E. 218 (1997) 71
- Rapakoulas, D., see Stamou, S. 218 (1997) 57
- Rayane, D., see Dugourd, Ph. 218 (1997) 163
- Reid, K.L., see Wouters, E.R. 218 (1997) 309
- Rettig, W., see Maus, M. 218 (1997) 151
- Rigler, R., see Mets, Ü. 218 (1997) 191
- Schael, F., J. Küster and H.-G. Löhmannsröben, The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates 218 (1997) 175
- Schmid, R.P., P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones, Infrared spectroscopy of aniline-X ( $\text{X} = \text{N}_2$ ,  $\text{CH}_4$ ,  $\text{CHF}_3$ ,  $\text{CO}$ ) clusters and their corresponding cluster cations in the  $\text{NH}_2$ -stretching vibration region 218 (1997) 291
- Shobatake, K., see Kanda, K. 218 (1997) 199
- Siebbeles, L.D.A., see Wouters, E.R. 218 (1997) 309
- Sinicropi, J.A., J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger, Hole transport in vapor deposited enamines and enamine doped polymers 218 (1997) 331
- Small, G.J., see Wu, H.-M. 218 (1997) 225
- Stamou, S., D. Mataras and D. Rapakoulas, Simulation of the  $\text{SiH}$  ( $\text{A}^2\Delta \rightarrow \text{X}^2\Pi$ ) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants 218 (1997) 57
- Stefanovich, E.V., see Truong, T.N. 218 (1997) 31
- Sugawara, K., see Schmid, R.P. 218 (1997) 291
- Swiatla-Wojcik, D., see Hawlicka, E. 218 (1997) 49

- Tabayashi, K., see Kanda, K. 218 (1997) 199
- Tajima, N., T. Taketsugu and K. Hirao, Theoretical study on adsorption and proton exchange reaction of H<sub>2</sub>O on H-form zeolite 218 (1997) 257
- Takeo, H., see Schmid, R.P. 218 (1997) 291
- Taketsugu, T., see Tajima, N. 218 (1997) 257
- Tan, K.H., see Olney, T.N. 218 (1997) 127
- Tanner, P.A., see Chua, M. 218 (1997) 83
- Tremblay, B., M.E. Alikhani and L. Manceron, Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study 218 (1997) 37
- Truong, T.N. and E.V. Stefanovich, Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential 218 (1997) 31
- Tyutyulkov, N., see Dietz, F. 218 (1997) 43
- Van der Zande, W.J., see Wouters, E.R. 218 (1997) 309
- Villarreal, P., see Buonomo, E. 218 (1997) 71
- Vinogradov, S.A., see Brunel, M. 218 (1997) 301
- Vojtík, J. and J. Fišer, Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH<sup>-</sup> and NeH<sup>+</sup> 218 (1997) 13
- Widengren, J., see Mets, Ü. 218 (1997) 191
- Wouters, E.R., L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande, Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H<sub>2</sub> 218 (1997) 309
- Wright, T.G., see Mack, P. 218 (1997) 243
- Wu, H.-M. and G.J. Small, Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores 218 (1997) 225
- Yang, B., see Guan, D. 218 (1997) 1
- Yang, S., see Hu, Y. 218 (1997) 325
- Yi, X., see Guan, D. 218 (1997) 1



## Subject index to volume 218

### Methods

#### Theoretical

##### *Group theory and algebras*

- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

##### *Many body and quasiparticle approaches*

- Thermodynamic shift from three- to two-dimensional systems, F. Cuadros, A. Mulero and W. Okrasinski 218 (1997) 235

##### *Ab initio schemes for stationary properties*

- Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH<sup>-</sup> and NeH<sup>+</sup>, J. Vojtík and J. Fišer 218 (1997) 13
- Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37
- Calculated thermodynamics of reactions involving NO<sup>+</sup>·X complexes (where X = H<sub>2</sub>O, N<sub>2</sub> and CO<sub>2</sub>), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243

##### *Computational and simulation methods*

- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43
- Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
- Simulation of the SiH (A<sup>2</sup>Δ → X<sup>2</sup>Π) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulis 218 (1997) 57

- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225
- Theoretical study on adsorption and proton exchange reaction of H<sub>2</sub>O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257
- Molecular dynamics and scattering theory*
- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
- A full quantum study of the vibrational predissociation mechanisms in Ar<sub>3</sub><sup>+</sup> cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
- Direct calculation of electronic Raman scattering intensity for Ce<sup>3+</sup> in Cs<sub>2</sub>NaCeCl<sub>6</sub>, M. Chua and P.A. Tanner 218 (1997) 83
- Experimental**
- Microwave spectroscopy*
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Infrared spectroscopy*
- Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37
- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277
- Infrared spectroscopy of aniline–X (X = N<sub>2</sub>, CH<sub>4</sub>, CHF<sub>3</sub>, CO) clusters and their corresponding cluster cations in the NH<sub>2</sub>-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
- Raman spectroscopy*
- Direct calculation of electronic Raman scattering intensity for Ce<sup>3+</sup> in Cs<sub>2</sub>NaCeCl<sub>6</sub>, M. Chua and P.A. Tanner 218 (1997) 83
- Visible and UV spectroscopy*
- Simulation of the SiH (A<sup>2</sup>Δ → X<sup>2</sup>Π) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulis 218 (1997) 57
- Quantitative studies of the photoabsorption and photoionization of PCl<sub>3</sub> in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127

- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Reverse saturable absorption in palladium and zinc tetraphenyltetraenzoporphyrin doped xerogels, M. Brunel, F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun 218 (1997) 301
- Fluorescence spectroscopy*
- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H<sub>2</sub>, E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309
- Electron impact spectroscopy*
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
- Laser methods*
- Direct calculation of electronic Raman scattering intensity for Ce<sup>3+</sup> in Cs<sub>2</sub>NaCeCl<sub>6</sub>, M. Chua and P.A. Tanner 218 (1997) 83
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
- Intermolecular vibrations of the van der Waals complex p-C<sub>6</sub>H<sub>4</sub>FCH<sub>3</sub>...Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325
- Synchrotron spectroscopies*
- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199
- Multiple resonance spectroscopy*
- Infrared spectroscopy of aniline-X (X = N<sub>2</sub>, CH<sub>4</sub>, CHF<sub>3</sub>, CO) clusters and their corresponding cluster cations in the NH<sub>2</sub>-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
- Atomic and molecular beam techniques*
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran-argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Intermolecular vibrations of the van der Waals complex p-C<sub>6</sub>H<sub>4</sub>FCH<sub>3</sub>...Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325



*Time-resolved experiments*

- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmansröben 218 (1997) 175
- Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331

*Mass spectrometry*

- Quantitative studies of the photoabsorption and photoionization of  $\text{PCl}_3$  in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Intermolecular vibrations of the van der Waals complex  $\text{p-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$ , Y. Hu, W. Lu and S. Yang 218 (1997) 325

*Field emission and field ionization*

- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211

**Objects****Bulk systems***Supersonic beams*

- A full quantum study of the vibrational predissociation mechanisms in  $\text{Ar}_3^+$  cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71

*Liquids neat*

- Thermodynamic shift from three- to two-dimensional systems, F. Cuadros, A. Mulero and W. Okrasinski 218 (1997) 235

*Liquid mixtures and solutions*

- Molecular dynamics simulation of NaCl solutions in methanol-water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49

*Crystals**-neat*

- Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43

*Glasses*

- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277



*Polymers*

- Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331

*Surfaces*

- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Theoretical study on adsorption and proton exchange reaction of H<sub>2</sub>O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257

*Plasmas*

- Simulation of the SiH ( $A^2\Delta \rightarrow X^2\Pi$ ) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57

*Biological systems*

- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

**Microscopic systems***Molecules (neutral and ionic)*

- Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Theoretical study on adsorption and proton exchange reaction of H<sub>2</sub>O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257

*-diatomic*

- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
- Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH<sup>-</sup> and NeH<sup>+</sup>, J. Vojtík and J. Fišer 218 (1997) 13
- Simulation of the SiH ( $A^2\Delta \rightarrow X^2\Pi$ ) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57
- Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H<sub>2</sub>, E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309

*-small polyatomics*

- Quantitative studies of the photoabsorption and photoionization of PCl<sub>3</sub> in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109

- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199
- aromatics*
- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277
- other large*
- Reverse saturable absorption in palladium and zinc tetraphenyltetraabenzoporphyrin doped xerogels, M. Brunel, F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun 218 (1997) 301
- Molecular aggregates*
- van der Waals molecules*
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran-argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Infrared spectroscopy of aniline-X ( $X = N_2, CH_4, CHF_3, CO$ ) clusters and their corresponding cluster cations in the  $NH_2$ -stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
- Intermolecular vibrations of the van der Waals complex  $p-C_6H_4FCH_3 \dots Ar$ , Y. Hu, W. Lu and S. Yang 218 (1997) 325
- clusters*
- Carbon-oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- A full quantum study of the vibrational predissociation mechanisms in  $Ar_3^+$  cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Infrared spectroscopy of aniline-X ( $X = N_2, CH_4, CHF_3, CO$ ) clusters and their corresponding cluster cations in the  $NH_2$ -stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291

*-complexes*

- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Calculated thermodynamics of reactions involving  $\text{NO}^+ \cdot \text{X}$  complexes (where  $\text{X} = \text{H}_2\text{O}$ ,  $\text{N}_2$  and  $\text{CO}_2$ ), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243

*Defects and impurities*

- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

*Ions and charge carriers*

- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31

**Phenomena***Molecular structure*

- Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267

*Vibrations and rotations of molecules*

- Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
- Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
- Intermolecular vibrations of the van der Waals complex  $\text{p-C}_6\text{H}_4\text{FCH}_3 \dots \text{Ar}$ , Y. Hu, W. Lu and S. Yang 218 (1997) 325

*Electronic structure and states*

- Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
- Simulation of the  $\text{SiH} (\text{A}^2\Delta \rightarrow \text{X}^2\Pi)$  emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulas 218 (1997) 57
- Direct calculation of electronic Raman scattering intensity for  $\text{Ce}^{3+}$  in  $\text{Cs}_2\text{NaCeCl}_6$ , M. Chua and P.A. Tanner 218 (1997) 83
- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199



*Electric and magnetic properties*

- Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH<sup>-</sup> and NeH<sup>+</sup>, J. Vojtík and J. Fišer 218 (1997) 13
- Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43

*Spin splittings*

- Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H<sub>2</sub>, E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309

*Optical activity*

- The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277

*Molecular interactions*

- Infrared spectroscopy of aniline-X (X = N<sub>2</sub>, CH<sub>4</sub>, CHF<sub>3</sub>, CO) clusters and their corresponding cluster cations in the NH<sub>2</sub>-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291

*Spectral bandshapes and intensities*

- Quantitative studies of the photoabsorption and photoionization of PCl<sub>3</sub> in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
- Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

*Energy transfer processes*

- Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1

*Molecular photophysical processes*

- Quantitative studies of the photoabsorption and photoionization of PCl<sub>3</sub> in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
- Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211

*Intramolecular dynamics**-vibrational energy redistribution (including vibrational dissociation)*

- A full quantum study of the vibrational predissociation mechanisms in  $\text{Ar}_3^+$  cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71

*Reactions (including dissociation)*

- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Calculated thermodynamics of reactions involving  $\text{NO}^+ \cdot \text{X}$  complexes (where  $\text{X} = \text{H}_2\text{O}$ ,  $\text{N}_2$  and  $\text{CO}_2$ ), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243
- Theoretical study on adsorption and proton exchange reaction of  $\text{H}_2\text{O}$  on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257

*-gas phase*

- Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199

*Electron transfer*

- The electronic structure of 4-(N,N-dimethylamino)-4'-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
- The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
- Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331

*Ionization (including Rydberg states)*

- Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
- Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211

*Fluctuations and noise*

- Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191

